How do you build a metal nanoparticle?

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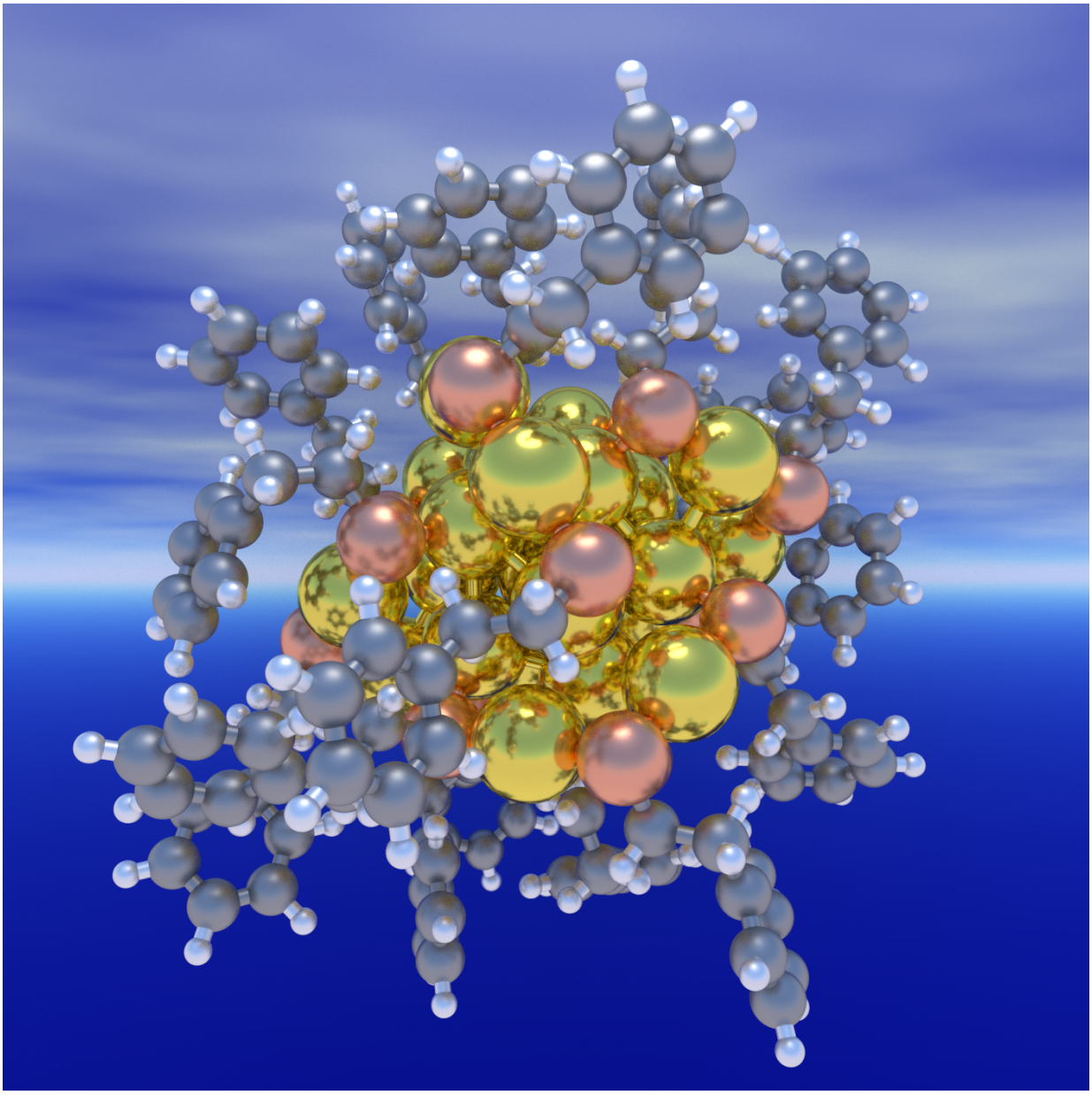

A structure of a ligand-protected Au25 nanocluster. Credit: Computer-Aided

Although scientists have for decades been able to synthesize nanoparticles in the lab, the process is mostly trial and error, and how the formation actually takes place is obscure. However, a study recently published in *Nature Communications* by chemical engineers at the University of Pittsburgh's Swanson School of Engineering explains how metal nanoparticles form.

"Thermodynamic Stability of Ligand-Protected Metal Nanoclusters" (DOI: 10.1038/ncomms15988) was co-authored by Giannis Mpourmpakis, assistant professor of chemical and petroleum engineering, and PhD candidate Michael G. Taylor. The research, completed in Mpourmpakis' Computer-Aided Nano and Energy Lab (C.A.N.E.LA.), is funded through a National Science Foundation CAREER award and bridges previous research focused on designing nanoparticles for catalytic applications.

"Even though there is extensive research into metal nanoparticle synthesis, there really isn't a rational explanation why a nanoparticle is formed," Dr. Mpourmpakis said. "We wanted to investigate not just the catalytic applications of nanoparticles, but to make a step further and understand nanoparticle stability and formation. This new thermodynamic stability theory explains why ligand-protected metal nanoclusters are stabilized at specific sizes."

A ligand is a molecule that binds to metal atoms to form metal cores that are stabilized by a shell of ligands, and so understanding how they contribute to nanoparticle stabilization is essential to any process of nanoparticle application. Dr. Mpourmpakis explained that previous theories describing why nanoclusters stabilized at specific sizes were

based on empirical electron counting rules - the number of electrons that form a closed shell electronic structure, but show limitations since there have been metal nanoclusters experimentally synthesized that do not necessarily follow these rules.

"The novelty of our contribution is that we revealed that for experimentally synthesizable nanoclusters there has to be a fine balance between the average bond strength of the nanocluster's metal core, and the binding strength of the ligands to the metal core," he said. "We could then relate this to the structural and compositional characteristic of the nanoclusters, like size, number of metal atoms, and number of ligands.

"Now that we have a more complete understanding of this stability, we can better tailor the nanoparticle morphologies and in turn properties, to applications from biolabeling of individual cells and targeted drug delivery to catalytic reactions, thereby creating more efficient and sustainable production processes."

More information: Michael G. Taylor et al, Thermodynamic stability of ligand-protected metal nanoclusters, *Nature Communications* (2017). DOI: 10.1038/ncomms15988

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